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The non-first-order factorizable contributions to the three–loop single mass operator matrix elements $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$

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Abstract

The non–first-order factorizable contributions to the unpolarized and polarized massive operator matrix elements to three–loop order, $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$, are calculated in the single mass case. For the ${}_2F_1$–related master integrals of the problem, we use the method of first–order differential equations for the master integrals in an arbitrary basis. Due to the singularity structure of the basis a part of the integrals has to be computed in the dimensional parameter to $O(\varepsilon^5)$. The solutions have to be matched at a series of thresholds and pseudo-thresholds in the region of the Bjorken variable $x \in]0, \infty[$ using highly precise series expansions to obtain the imaginary part of the physical amplitude for $x \in]0, 1]$ at a final relative accuracy of $O(10^{-10})$ or better. We compare the present results both with previous analytic results, the results for fixed moments in Mellin N, and a prediction in the small x region. We also derive expansions in the region of small and large values of x. Herewith all three–loop single mass unpolarized and polarized operator matrix elements are calculated.

1 Introduction

The heavy flavor corrections both to the deep–inelastic unpolarized and polarized structure functions form an essential part of these quantities. Their scaling violations are different than those of the massless contributions. Since the experimental precision reached the 1% level in the unpolarized case with HERA [1], which will also be the case for polarized deep–inelastic scattering at EIC [2] and later at the LHeC [3], the three–loop heavy flavor corrections are needed.

In a previous paper [4] we have calculated the first-order factorizable contributions to the constant part of the unrenormalized three–loop massive operator matrix elements (OMEs) $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$, $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$, which are based on 1009 of a total of 1233 Feynman diagrams in the unpolarized case. For all contributions 1000 or more non–vanishing Mellin moments are know. Furthermore, 15 of the 25 color–ζ contributions to the OMEs have been calculated by using the method of arbitrarily high Mellin moments [5]. Their associated recurrences were computed by using the guessing method [6,7] and solved by the package `Sigma` [8,9] in all first order factorizing cases.

The major new aspect of the present calculation is the contribution of higher transcendental letters in the iterated integrals forming the master integrals given by ${}_2F_1$–solutions [10] [1] of Heun differential equations [20, 21]. The corresponding basic integrals have been computed to $O(\varepsilon^0)$ in Ref. [22]. Here $\varepsilon = D - 4$ denotes the dimensional parameter. The other master integrals are obtained by iterating Kummer–Poincaré [23–32] and square–root valued letters [4, 33], by which all master integrals can be obtained.

In the present paper we start with the first–order differential equation system of master integrals, obtained by the integration by parts (IBP) reduction [34, 35]. The solution of these equations is performed in t–space [36,37]. After analytic continuation from t to x–space, cf. [22], the initial conditions are given at $x \to \infty$ as the Mellin moments to the requested order in ε. In our set of master integrals one has to calculate up to $O(\varepsilon^5)$ in individual cases. The initial values have been computed already before for determining the corresponding recurrences in Mellin–N space, cf. [4]. The analytic continuation has to pass a series of pseudo–thresholds and thresholds from $x \to \infty$ to $x = 0$ and matching conditions have to be evaluated. The present approach uses large mantissa rational matching in this process. At any of the expansion point we maintain 100 terms, except for $x = 1$ and $x = 0$, where also logarithmic terms contribute. Here we compute 50 terms. All constants emerging are evaluated to 250 digits. In this way we finally obtain the constant parts of the unrenormalized massive OMEs $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$, $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$. This formalism is only applied to the part of the amplitude which is affected by ${}_2F_1$–related letters.[2]

The paper is organized as follows. In Section 2 we describe the basic computation method. In Section **??** we compute $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$ in x–space, compare to previous partial results in the literature, and present numerical results. The results for small and large values of Bjorken x are presented in Section 3 and Section 4 contains the conclusions.

2 The main steps of the calculation

The calculation of the contributing Feynman diagrams for their generation to the reduction of the master integrals have been described in Ref. [4]. Here we use the packages `QGRAF, Form, Color`

[1] They are related to complete elliptic integrals and modular forms, cf. Refs. [11–18] and the surveys in Ref. [19].

[2] Later work will be devoted to the method of iterating non–iterative integrals, including higher transcendental letters.

and Reduze 2 [34, 35, 38–41], using the Feynman rules given in Refs. [42, 43]. In the polarized case we compute the OME in the Larin scheme [44]. The OMEs are calculated using the method described in Ref. [22] starting with a generating function for the Mellin moments at discrete integer values of N by a continuous real variable t. The master integrals are computed in this variable by solving linear systems of differential equations, cf. also Refs. [4, 45–47]. The initial values are provided by the Mellin moments [48], which are the expansion coefficients at $t = 0$. The system of differential equations is solved at a series of thresholds and pseudo–threshold in the region $t \in [0, \infty[$. The variables t and the Bjorken variable x are related by

$$x = \frac{1}{t}. \tag{2.1}$$

The set of thresholds and pseudo–thresholds in the differential equations of all master integrals, resp. the necessary expansion points, given the convergence radius of the respective local series, are

$$\left\{\frac{1}{32}, \frac{9}{50}, \frac{17}{50}, \frac{59}{100}, \frac{71}{100}, \frac{15}{19}, \frac{80}{93}, 1\right\} \tag{2.2}$$

in x in the present problem. Imaginary parts for the amplitude are developed only at the transition point $x = 1$, and for no other points in the regions $x \in]0, 1[$ and $x \in]1, \infty[$. The thresholds for $x > 0$ were

$$\left\{\frac{8}{7}, \frac{4}{3}, 2, 4, \infty\right\}. \tag{2.3}$$

The analysis starts at $x = \infty$ using the initial values there, which are needed to a certain order in ε, depending on the set of master integrals. In the present case one needs to expand up to $O(\varepsilon^5)$ in some cases. One performs series expansions around the (pseudo)thresholds. These are matched in the middle between two expansions at 250 digits. The corresponding numbers are rationalized, which allows a faster solution of the linear equation systems. In the calculation of the series expansions the linear equations are solved with FireFly [49, 50] using modular methods. In all expansions we also expand in the dimensional parameter ε. Except of the points $x = 0$ and $x = 1$ we compute 100 expansion coefficients, while at the latter points, which contain in addition powers of the logarithms $\ln(x)$ and $\ln(1 - x)$, respectively, 50 expansion terms are used.

The initial values at $x \to \infty$ are real as also the coefficients of the linear differential equation systems. For the expansion points for $x > 0$ the series expansions are real–valued Laurent series in x and their contribution to the massive OMEs vanish, cf. [22]. The analytic continuation at $x = 1$ implies logarithmic–modulated series containing powers of $\ln^k(1 - x)$ and such an imaginary part, leading to finite contributions to the massive OMEs.

3 $a_{Qg}^{(3)}(x)$ and $\Delta a_{Qg}^{(3)}(x)$

In Ref. [4] we computed all color–ζ contributions, which can be obtained by solving difference equations which factorize at first order. Furthermore, we calculated all remaining irreducible Feynman diagrams with contributions of master integrals, the differential equations of which, factorized also at first order. The remaining 224 Feynman diagrams are related to ${}_2F_1$–solutions [10, 22] and are calculated in the present paper by solving the first order differential equations obtained from the IBP–relations directly in a highly precise numerical approach, adding the previous results to the complete solution.

There are also reducible Feynman diagrams and ghost contributions to the amplitudes $A_{Qg}^{(3)}(x)$ and $\Delta A_{Qg}^{(3)}(x)$, contributing to the final result, which we would like to characterize briefly.In the unpolarized case in Mellin N-space they are spanned by the harmonic and generalized harmonic sums [32, 51, 52]

$$\Big\{S_{-4}, S_{-3}, S_{-2}, S_1, S_2, S_3, S_4, S_{-3,1}, S_{-2,1}, S_{-2,2}, S_{3,1}, S_{2,1}, S_{2,1,1}, S_{-2,1,1}, S_1\left(\left\{\frac{1}{2}\right\}\right), S_1(\{2\}), S_{1,3}\left(\left\{\frac{1}{2}, 2\right\}\right), S_{2,1}(\{1,2\}), S_{2,1}(\{2,1\}), S_{1,1,1}(\{2,1,1\}), S_{1,1,2}\left(\left\{\frac{1}{2}, 2, 1\right\}\right), S_{1,2,1}\left(\left\{\frac{1}{2}, 2, 1\right\}\right), S_{1,1,1,1}\left(\left\{\frac{1}{2}, 2, 1, 1\right\}\right)\Big\} \tag{3.1}$$

with rational prefactors. In x–space these terms convert to harmonic polylogarithms [53] at argument x or $1-2x$, like in Ref. [54]. The generalized sums stem from the ghost contributions, which are absent in the polarized case.

Expanding their contribution around $x = 0$ terms of order

$$\frac{\ln^4(x)}{x}, \quad \frac{\ln^3(x)}{x}, \quad \frac{\ln^2(x)}{x} \tag{3.2}$$

with

$$C_A^2 T_F \frac{1}{z}\left[\frac{1}{54}\ln^4(z) + \frac{1}{18}\ln^3(z) + \left(\frac{61}{36} + \frac{1}{3}\zeta_2\right)\ln^2(z)\right], \tag{3.3}$$

are present, which are not expected in the complete result. Indeed the calculation shows, that these terms are canceled at a relative accuracy of

$$\left\{-2.7134 \cdot 10^{-17}, -1.1975 \cdot 10^{-13}, -1.4327 \cdot 10^{-15}\right\} \tag{3.4}$$

in the complete result numerically. Contributions of this kind do not emerge in the polarized case.

Our present results can be tested also in various other ways. Next we compare the result in x space with the moments computed in Ref. [43] by a totally different method, using `MATAD` [55]. For the moments $N = 2, 4, 6, 8, 10$ we obtain relative accuracies of

$$\left\{-4.3039 \cdot 10^{-8}, 1.0758 \cdot 10^{-9}, 6.9438 \cdot 10^{-10}, -4.3401 \cdot 10^{-11}, -1.4872 \cdot 10^{-10}\right\} \tag{3.5}$$

in the unpolarized case. Since the first moment of $\Delta a_{Qg}^{(3)}$ turns out to be zero, we compare here the relative deviation of the moments $N = 3, 5, 7, 9, 11$, for which we obtain

$$\left\{-8.9221 \cdot 10^{-10}, 9.6270 \cdot 10^{-10}, -2.4977 \cdot 10^{-10}, -1.7849 \cdot 10^{-10}, 3.1817 \cdot 10^{-11}\right\}. \tag{3.6}$$

A further test of accuracy consists in the comparison of the present differential equation method with the analytic results obtained by N–space techniques on the N_F terms to $a_{Qg}^{(3)}(x)$ and $\Delta a_{Qg}^{(3)}(x)$ before. For

$$(\Delta)r(x) = \frac{(\Delta)a_{Qg}^{(3),\mathrm{deq}}(x)}{(\Delta)a_{Qg}^{(3),\mathrm{ex}}(x)} - 1 \tag{3.7}$$

we obtain

$$x \rightarrow \left\{\frac{1}{100}, \frac{1}{10}, \frac{3}{10}, \frac{5}{10}, \frac{7}{10}, \frac{9}{10}, \frac{99}{100}\right\}, \tag{3.8}$$

$$r(x) \rightarrow \Big\{2.22 \cdot 10^{-16}, -7.77 \cdot 10^{-16}, -1.75 \cdot 10^{-14}, -5.11 \cdot 10^{-15}, -2.11 \cdot 10^{-15}, -2.72 \cdot 10^{-13}, 1.11 \cdot 10^{-15}\Big\}. \tag{3.9}$$

$$\Delta r(x) \rightarrow \Big\{5.40 \cdot 10^{-14}, 8.40 \cdot 10^{-11}, -6.40 \cdot 10^{-10}, 4.07 \cdot 10^{-10}, -7.25 \cdot 10^{-10}, 9.31 \cdot 10^{-8}, -5.90 \cdot 10^{-9}, \Big\}. \tag{3.10}$$

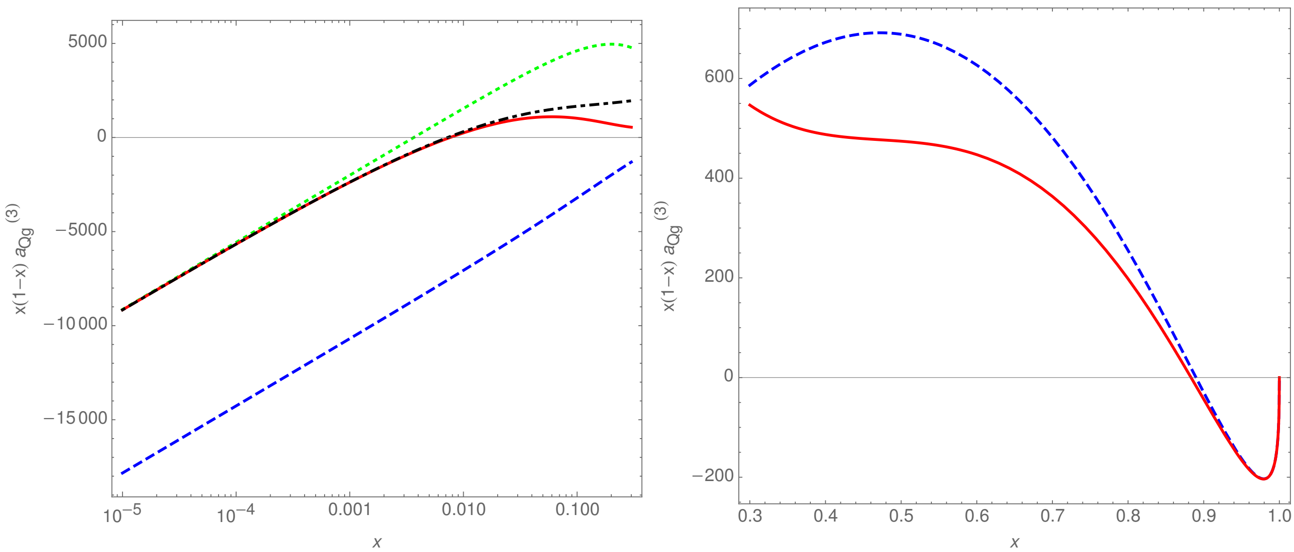

Figure 1: $a_{Qg}^{(3)}(x)$ as a function of x rescaled by the factor $x(1-x)$. Left panel: smaller x region. Full line (red): $a_{Qg}^{(3)}(x)$; Dashed line (blue): leading small x term $\propto \ln(x)/x$ [56]; Dotted line (green): $\ln(x)/x$ and $1/x$ term; Dash-dotted line (black): all small x terms up to $\ln^5(x)$. Right panel: larger x region. Full line (red): $a_{Qg}^{(3)}(x)$; Dashed line (blue): leading large x terms up to the terms $\propto (1-x)$, covering the logarithmic contributions of $O(\ln^k(1-x))$.

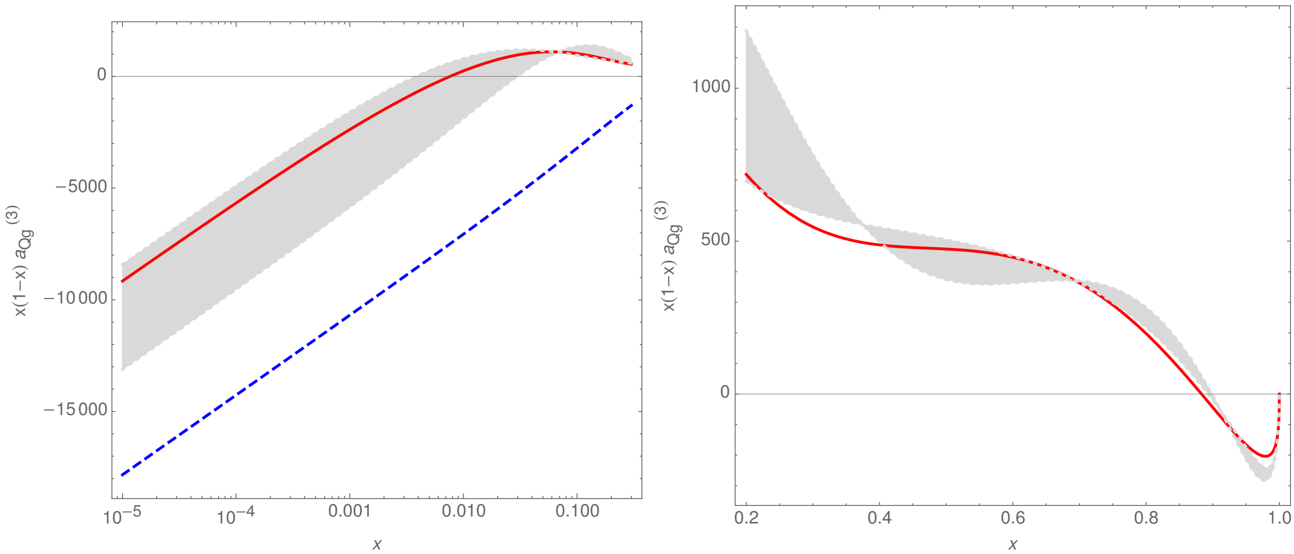

Figure 2: $a_{Qg}^{(3)}(x)$ as a function of x rescaled by the factor $x(1-x)$. Left panel: smaller x region. Full line (red): $a_{Qg}^{(3)}(x)$; Dashed line (blue): leading small x term $\propto \ln(x)/x$ [56]; Gray region: estimates of [61]. Right panel: larger x region. Full line (red): $a_{Qg}^{(3)}(x)$; Gray region: estimates of [61].

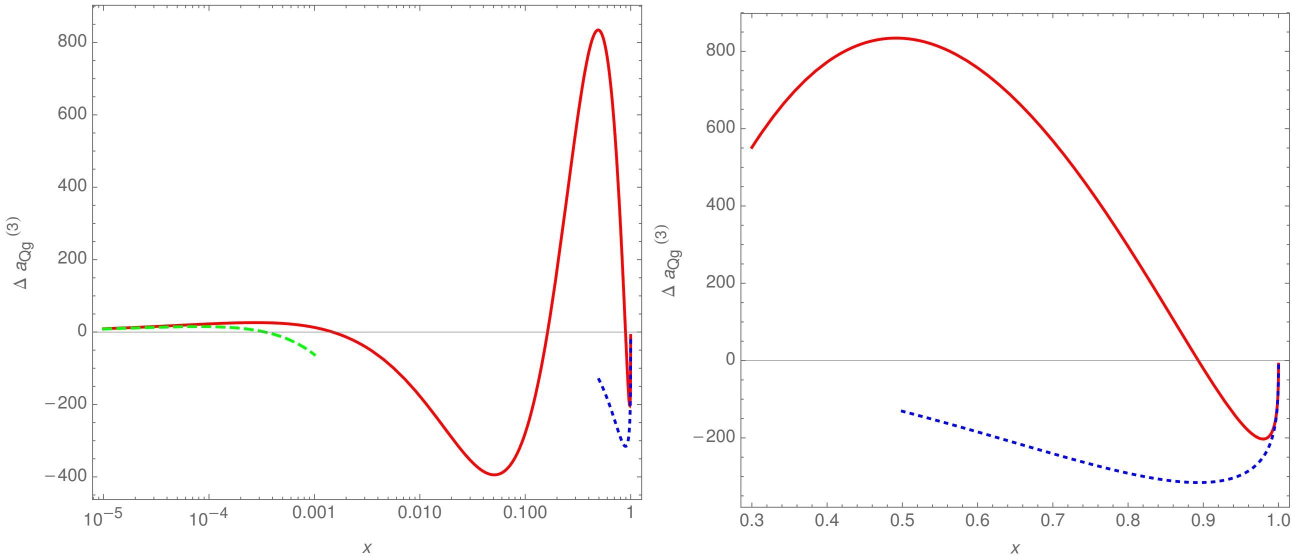

Figure 3: $\Delta a_{Qg}^{(3)}(x)$ as a function of x rescaled by the factor $x(1-x)$. Left panel: Full line (red): $\Delta a_{Qg}^{(3)}(x)$; Dashed line (green): the small x terms $\ln^k(x), k \geq 1$; Dotted line (blue): the large x terms $\ln^l(1-x), l \geq 1$. Right panel: larger x region. Full line (red): $\Delta a_{Qg}^{(3)}(x)$; Dotted line (blue): the large x terms $\ln^l(1-x), l \geq 1$.

For smaller values of x the deviations are even smaller. A comparable accuracy has also been obtained for the pole terms of the unrenormalized amplitudes $A_{Qg}^{(3)}(x)$ and $\Delta A_{Qg}^{(3)}(x)$ which are also known in analytic form.

Now we turn to the results on $a_{Qg}^{(3)}(x)$ and $\Delta a_{Qg}^{(3)}(x)$ In Figures 1 and 2 we illustrate the analytic result for $a_{Qg}^{(3)}(x)$ for QCD and by setting $N_F = 3$ in the region $x \in [0,1]$ and in the region of larger values of x only. Here we add different lines for the small x and large x contributions to show their validity. The so-called leading small x result [56] turns out to not to describe the physical quantity $a_{Qg}^{(3)}(x)$ quantitatively; see, however, the discussion in Section 3. This is, as in all known other cases, see e.g. [54, 57–60], due to sub–leading terms which cancel the leading behaviour. Here the inclusion of the $1/x$ term, not predicted by small x methods, leads to a description up to $x \sim 10^{-4}$. To describe the region to $x \sim 2 \cdot 10^{-2}$ one needs also all contributing $\ln^k(x), \quad k \geq 1$ terms. In the large x region no expansion terms have been predicted. Here one obtains a description to $x \sim 0.9$ by considering all $\ln^k(1-x)$ terms for $k \geq 0$ and the $(1-x)$ contributions.

In Ref. [61] estimates on the size of the charm quark contributions in $F_2(x, Q^2)$ were made based on five moments for $A_{Qg}^{(3)}$ and six moments for $A_{Qq}^{(3),\rm PS}$ calculated in Ref. [43], the two–loop contributions of Refs. [62, 63], and the N_F-terms from our calculation Ref. [64], as well as by assuming the small x behaviour from [56] for $A_{Qg}^{(3)}$ and a corresponding color–rescaled leading small–x term for $A_{Qq}^{(3),\rm PS}$.

The latter has been first proven in Ref. [54] by calculating $A_{Qq}^{(3),\rm PS}$ in complete form analytically. In [61] the three other contributing OMEs $A_{qg,Q}^{(3)}$, $A_{qq,Q}^{(3),\rm NS}$, $A_{qq,Q}^{(3),\rm PS}$, as well as the two–mass corrections, were not taken into account. In Figure 2 we illustrate the former estimate on $a_{Qg}^{(3)}(x)$ in the region of smaller and larger values of x (gray band) and compare it to the exact result (red lines), laying close to the upper end of the former estimate in the region of small values of x.

Let us now turn to the polarized case. $\Delta a_{Qg}^{(3)}(x)$ is shown in Figure 3. We indicate also the small and large x terms, cf. Section 4. They describe only extreme regions. $\Delta a_{Qg}^{(3)}(x)$ shows an oscillatory behaviour as also known for the polarized structure functions $g_{1,2}(x, Q^2)$. In the present case one reason is, that the first moment of $\Delta a_{Qg}^{(3)}(x)$ vanishes. This is also for the first and second orders in the strong coupling constant, cf. [65].

4 The small and large x limits

The leading small–x contribution to the unpolarized quantity $a_{Qg}^{(3)}(x)$ has been predicted in Ref. [56], within a leading order calculation based on $k_\perp$–factorization, by

$$a_{Qg}^{(3),x\to 0}(x) \quad = \quad \frac{64}{243} C_A^2 T_F \left[1312 + 135\zeta_2 - 189\zeta_3\right] \frac{\ln(x)}{x}. \tag{4.1}$$

As we saw in Section 3 this result is interesting for the theoretical comparison to the corresponding term in the complete calculation, but cannot be used for phenomenology due to the destructive subleading corrections. We obtained the term $\propto \zeta_2$ in Ref. [4] since it results from first order factorizing contributions only. From the small x expansion of the present result we obtain an agreement on the purely rational and ζ_3 term of Eq. (4.1) at a relative accuracy of

$$\{-8.0143 \cdot 10^{-16}\}. \tag{4.2}$$

This is the first independent recalculation of the result of [56] by using a different method and it also establishes the rescaling to the corresponding analytic result in the pure singlet case [54].

The small x terms for $a_{Qg}^{(3)}$ are given numerically by[3]

$$a_{Qg}^{(3),x\to 0} \quad \simeq \quad 1548.891667 \frac{\ln(x)}{x} + [8999.437146 - 102.4674542 N_F] \frac{1}{x}$$

[3]Here we present 10 digits for brevity, although our result is more accurate.

$$
\begin{aligned}
&+ \quad [4.844444444 - 0.4444444444 N_F] \ln^5(x) \\
&+ \quad [-23.09259259 - 2.061728395 N_F] \ln^4(x) \\
&+ \quad [509.6468278 - 33.72805463 N_F] \ln^3(x) \\
&+ \quad [-755.5219042 - 79.02963486 N_F] \ln^2(x) \\
&+ \quad [10748.66273 - 471.2333706 N_F] \ln(x). \qquad (4.3)
\end{aligned}
$$

The alternating sign of the first two coefficients is the main reason why the leading small x contributions lays off the final result. For a precise description also the further subleading terms are needed.

In the large x limit $a_{Qg}^{(3)}$ is given by

$$
\begin{aligned}
a_{Qg}^{(3),x\to 1} &\simeq 3.703703704 \ln^5(1-x) + [-8.20987654 + 0.4938271605 N_F] \ln^4(1-x) \\
&+ [4.380199906 + 1.646090535 N_F] \ln^3(1-x) \\
&+ [-332.5368214 - 0.4183246058 N_F] \ln^2(1-x) \\
&+ [737.165347 - 73.1297935 N_F] \ln(1-x). \qquad (4.4)
\end{aligned}
$$

In the polarized case the leading small x terms are

$$
\begin{aligned}
\Delta a_{Qg}^{(3),x\to 0} &\simeq [-12.60493827 + 0.4444444444 N_F] \ln^5(x) \\
&+ [-145.2160494 + 7.839506173 N_F] \ln^4(x) \\
&+ [-856.9645724 + 63.82682006 N_F] \ln^3(x) \\
&+ [-852.7889255 + 298.2461398 N_F] \ln^2(x) \\
&+ [25006.51309 + 544.6633205 N_F] \ln(x). \qquad (4.5)
\end{aligned}
$$

Here the coefficients of the terms $\ln(x)/x$ and $1/x$ haven been shown to be zero in [4]. The N_F term $\propto \ln^5(x)$ has been derived in Ref. [4] as $C_F T_F^2 N_F (4/3) \ln^5(x)$. The coefficients in (4.6) are alternating.

The expansion coefficients in the large x region are

$$
\begin{aligned}
\Delta a_{Qg}^{(3),x\to 1} &\simeq 3.703703704 \ln^5(1-x) + [-8.20987654 + 0.49382716105 N_F] \ln^4(1-x) \\
&+ [4.380199906 + 1.646090535 N_F] \ln^3(1-x) \\
&+ [-332.5368214 - 0.4183246058 N_F] \ln^2(1-x) \\
&+ [737.165347 - 73.1297935 N_F] \ln(1-x). \qquad (4.6)
\end{aligned}
$$

The large x expansions are the same in the unpolarized and polarized case. These results were derived in two different calculations.

5 Conclusions

We have calculated the non-first-order factorizable contributions to the three–loop massive operator matrix elements $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$. This completed the computation of these matrix elements and herewith of all of the three–loop single mass unpolarized and polarized OMEs [4,54,64,66–72]. Also the two–mass corrections [73–78] except those for $(\Delta) A_{Qg}^{(3)}$ have already been computed. The solution of the first order differential equation system of master integrals in different sub–intervals of $x \in]0, \infty[$ at very high numerical precision and high precision matching using the methods [22, 45] allowed to derive the three–loop corrections tied up to iterative non–iterative integrals containing ${}_2F_1$–letters in terms of local series expansions. The latter are logarithmic–modulated with powers of $\ln(x)$ around $x = 0$ and $\ln(1-x)$ around $x = 1$.

We confirm the leading small x prediction for the $O(\ln(x)/x)$ term in the unpolarized case in an independent calculation using a different method for the first time. We compared our results with the moments [43] and other terms, which were calculated by us by different methods and found agreement. The present results are important for future measurements of the strong coupling constant $\alpha_s(M_Z^2)$ [79–82], the charm quark mass, m_c, [83] and the parton distribution functions, cf. e.g. [84, 85]. The three loop single–and two–mass corrections to deep–inelastic scattering will be released in form of a numerical code in another publication.

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